Integrating Best Practice Pedagogy with Computer-Aided Modeling and Simulation to Improve Undergraduate Chemical Engineering Education

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Abstract: This paper presents an undergraduate Course, Curriculum and Laboratory Improvement project at the Chemical Engineering Department, Lamar University, funded by the US National Science Foundation. This project combines the problem-based learning pedagogy with extensive use of computer-aided modeling and simulation packages. The approach used here is to examine the entire chemical engineering curriculum, integrate the use of "hands-on" computer-aided modeling and simulation packages into the entire range of courses, and involve the student, teacher, and industry in bringing this to fruition. The Accreditation Board of Engineering and Technology Engineering Criteria 2000 framework will be followed to evaluate the outcome from this project. The reform process will have a beneficial effect on both the teachers and the students of the Chemical Engineering undergraduate curriculum. Computer packages such as HYSYS, PRO/II, ASPEN Plus, POLYMATH and Gaussian are employed in nine Chemical Engineering courses. POLYMATH is used in several undergraduate classes to permit students to obtain numerical solutions to problems that are difficult to solve analytically. Examples in Momentum Transfer, Heat Transfer, and Kinetics are presented. HYSYS is utilized to operate a flash vaporization and test the effects of pressure and preheating. Dynamics and control of a propylene glycol plant are analyzed by Process Control students using HYSYS, which has an integrated steady-state and dynamic simulation environment. Various control schemes are studied and the dynamic performance is evaluated. A preliminary design for silane production is covered in Process Design class. This creative design utilizes computer-aided modeling and simulation packages in preparing the design, including raw material requirements, energy requirements, list of major process equipment, and process economics.

Keywords: problem-based learning, computer-aided modeling and simulation

Introduction

Lamar University is located at the center of Spindletop, which was the site of the first gusher in Texas and, hence, where the petroleum refinery and petrochemical industry in the United States began [1]. In the past forty years or so, the faculty in the Chemical Engineering Department at Lamar, like the faculty at almost all universities, taught the classes by preparing the notes, lecturing in the classes, and giving tests to the students. We hoped that our students graduated with good problem solving skills. Yet, we observed a big gap between this goal and the real situation. Feedback from our alumni, comments from industry, and discussions among our faculty members urged the Chemical Engineering Department at Lamar to adapt and implement the problem-based learning (PBL) pedagogy [2] with extensive use of computer-aided modeling and simulation (CAMS) packages to modernize and improve our chemical engineering undergraduate teaching. This extensive teaching improvement has received full support from the US National Science Foundation's undergraduate Course, Curriculum and Laboratory Improvement (CCLI) program.

Over the past forty years, the development of digital computers has had the most influence on our lives, including engineering practicing and teaching. Mathematical modeling and simulation are important and useful areas of computer application. Thirty years ago engineers in industry were skeptical of computer simulation as a valid way to solve manufacturing problems. However, today the prevailing view in industry is that running simulations is much less expensive and more reproducible than performing repeated experiments [3]. Through the use of CAMS, the extension of traditional teaching strategies can be more practical and efficient, and genuinely new strategies can be made possible. In reality, the use of CAMS packages in a reformed chemical engineering curriculum may provide an in-depth understanding of the basics of chemical engineering and at the same time develop the skills to use the packages properly. The development of teaching and research strategies can be enhanced tremendously by adopting and adapting these new developments and building on the accomplishments of others in creative problem solving [4] and in advanced teaching methods that impact quality [5].

Our primary objective is to use CAMS packages, through learning principles and realistic problem practices, to provide accelerated exposure to PBL. This plan provides an innovative adaptation and implementation of the concepts of integrated, problem-based, interdisciplinary pedagogical principles. A secondary objective is to adopt commercial modeling software packages, such as HYSYS, PRO/II, ASPEN Plus, and POLYMATH, in each selected course. These software packages will not be used as "black boxes" or mere tools from which to extract solutions, but will be used to enhance the fundamental understanding of the principles on which modeling and simulation tools are based. In summary the goal is to integrate the learning of traditional, conventional engineering principles with latest computer technology in direct application to real-world problem solving in order to train practical and knowledgeable chemical engineers who can quickly attain an effective functioning level in industries that depend increasingly on CAMS.

The figure below gives the approach and scope of the original CCLI project, which has three phases. The

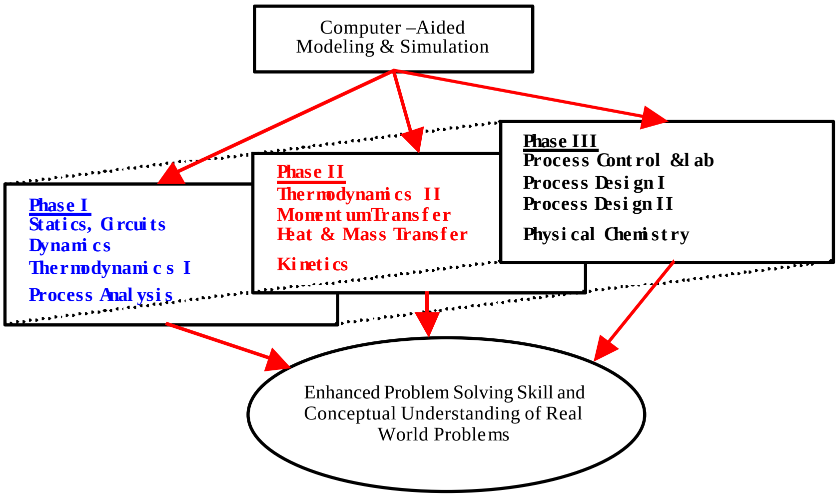

Fig. 1. Three phases for the CCLI project

courses are divided among these phases to allow full development and assessment of the program. The product will be a chemical engineering training program that graduates students with enhanced problem-solving skills, particularly with CAMS, and an exceptional conceptual understanding of real-world problems.

Examples of CAMS implementation in Kinetics, Momentum Transfer, Heat Transfer, Mass Transfer, Process Control, and Process Design are given in the following sections.

Kinetics

In the undergraduate Reaction Kinetics class, the students used POLYMATH [6] extensively to solve three types of problems. The first type asked the students to use linear, polynomial, and/or nonlinear regression to fit experimental data to rate laws to determine best-fit values for the rate law parameters. The second type required the students to solve systems of nonlinear equations to analyze multiple steady states and hysteresis in continuous stirred-tank reactors. The third type asked the students to solve systems of nonlinear ordinary differential equations to model two classes of systems: those containing multiple chemical reactions and those used to analyze nonisothermal gas-phase reactions in packed bed reactors.

A good example of this last class of problem is Fogler's Problem 8-7 [7] which asks the students to plot the temperature, conversion, and pressure versus weight of catalyst down the length of the reactor. The reaction in question is the elementary, irreversible, exothermic, gas-phase decomposition $A \rightarrow B + C$, which occurs in an adiabatic reactor packed with catalyst. To solve the problem, the students first obtained two coupled nonlinear ordinary differential equations: one for conversion as a function of catalyst weight derived from the design equation of a packed bed reactor, the other for pressure as a function of catalyst weight derived from the Ergun equation [8]. They next combined these two differential equations with algebraic equations derived from the energy balance (which relates the temperature in the reactor to the conversion), the rate law, and stoichiometry. Finally, they used the ordinary differential equation solver in POLYMATH to obtain the requested plots.

The three types of problems mentioned above can be divided into two categories: those that cannot be solved analytically, and those that can. For the first category, the advantage of using a computer is manifest: the students cannot otherwise obtain a solution. For the second category, allowing the students to use a computer still presents one main advantage: they can focus on getting the solution rather than on learning the sometimes arcane techniques required to obtain the analytic solution. One quintessential example of this is the problem of finding the roots of a cubic equation. The general analytic solution has been known since the 16th Century [9] but it is rarely used to solve the problem unless the emphasis is on the method rather than the solution. Thus, in the undergraduate Reaction Kinetics class the students made extensive use of POLYMATH to solve problems both on the homework and on the exams.

Momentum Transfer

One potential application of the computer-aided approach in the Momentum Transfer course is to employ commercial packages to simulate pressure drop profiles associated with specific pipe-line designs. In the past, students were assigned to write their own computer programs to simulate the process, which usually involved the inclusion of all the necessary equations to estimate pressure drop and friction factors for various components and under various operating conditions. The practice was time-consuming and the reliability was poor. With the adoption of commercial packages such as HYSYS [10] for such applications, the burden of programming is substantially reduced and students will be able to focus on the effects of various parameters on the simulation results.

Heat Transfer

An interesting design problem in undergraduate Heat Transfer is the calculation of heat loss through flanges on a steel pipe. The system equation, a second-order ordinary differential equation derived from an energy balance around the flanges, is a modified Bessel equation. The analytical solution may be obtained by using two boundary conditions: one is the constant temperature at the pipe wall and the other is the conduction rate is equal to the convection rate at the flange rim. The derivation is tedious and the solution equation is enormous [11]. Quite often, the students are lost before coming to the calculation of the heat loss through the flanges. Nowadays, the students can use POLYMATH to solve this second-order ordinary differential equation (watch for the two-point boundary value instead of initial value problem). With the help of this powerful computer package, the students have extra time to try different values of the heat transfer coefficient and see its effect on the total heat loss. The students can enjoy the interpretation of the calculation results now.

Mass Transfer

In the undergraduate Mass Transfer class, mass transfer principles are first studied and then mass transfer unit operations such as flash vaporization, absorption, and distillation are covered for both binary and multi-component systems. Although the binary system is important for concept teaching, the learning of the multi-component system is a must in the real world. In the past, the students had to write their own computer programs to solve mass and energy balance for their multi-component non-isothermal equilibrium-stage design homework. A simple but good example is the adiabatic flash vaporization of a multi-component hydrocarbon mixture to find the temperature and compositions of vapor and liquid phases at equilibrium [12]. Combining the calculation methodology with the thermodynamic properties predictions makes this type of computation very tedious and time-consuming. Quite often, the students have to spend several days in programming and debugging; therefore, they do not have time to interpret the results. Now, using computer packages such as HYSYS, ASPEN [13], and PROII [14], the students can obtain the solution within a few hours (if not minutes). The students even have time to change the pressure of the flash drum or add a preheater to the feed stream and see their effects on separation of a key component.

Another example is absorption tower design for a multi-component gas absorption under adiabatic condition. Again, in the past the students had to spend several days developing their computer programs to calculate the concentration and temperature distributions for the entire absorption tower. These days, with the help of commercial computer simulation package, students can have the solution within an hour. The students can then change the design parameters such as flow rates and tower pressure to see the absorption percent of a specified component in the gas stream. The students even have an opportunity to input the tray efficiency to examine the results of a non-ideal tray by using these modern simulation packages.

Process Control

The Process Control class covers fundamentals of process dynamics, PID feedback control, and advanced model-based, multivariable control [15-17]. The Process Control Laboratory at Lamar University consists of three analog units for level, flow, and temperature control (donated by Fisher/Scallon Controls), a pH adaptive control unit, a Schweitzer Heat Exchanger/Thermal Mixing unit, an Atlantic Distillation Process Simulator (sponsored by Dow chemical), ISA PID Tuning software, and a HYSYS dynamic process simulator [18,19]. The Process Control Laboratory class provides indispensable learning experience to our senior students. Updated process dynamics software, ASPEN Dynamics and ASPEN Custom Modeler [20], are being purchased for the Process Control class.

At this point, we have used HYSYS in our Process Control Laboratory as a lab unit for learning process dynamics and basic/enhanced PID control. HYSYS is widely used in the chemical process and natural gas industries. Familiarity with HYSYS is a valuable, marketable skill for chemical engineering graduates. The package has the distinct advantage of integrating the dynamic and the steady state simulations into one. As a result, students can run the propylene glycol steady state flowsheet and then use the results as the initial conditions for dynamic simulation when a disturbance is encountered [10]. The process simulator helps students learn how the controllers work by examining responses from the strip charts in the same way that engineers and operators examine responses on a console in a plant control room.

In this exercise, a flowsheet for the production of propylene glycol is presented. Propylene oxide is combined with water to produce propylene glycol in a CSTR. The reactor products are then fed to a distillation tower, where essentially all the glycol is recovered in the tower bottoms. The students are asked to maintain the process at the desired operating conditions. Two dynamic simulations are studied: a drop of the reactor set point from 140 to 125^{o}F, and a return to the original set point using the controller ramp feature. As mentioned earlier, historical data can be viewed in the strip charts and stored as a data file. The strip charts allow students to monitor the response of the reactor itself, as well as how the change propagates downstream to the distillation tower. All actions required can be completed within a reasonable time period (three hours each week for two weeks). Students are required to submit a lab report a week after the lab is completed.

Process Design

Process Simulation is utilized in the senior design course. The unit operations encompassed in the process simulation cover the following: cooler/heater, 2-phase separator (vapor-liquid), 3-phase separator (vapor-liquid I-liquid II), fractionator, heat exchanger, mass balance reactor, mixer, pipe segment, multiple pipe segments and mixer, turbo-expander plant (high-pressure phase separator, expander, low pressure phase separator, and distillation with 2 feeds), and flare system (multiple inlets, multiple mixer, and common flare).

A plant design project is also covered in the course. A preliminary process design for the production of silane is covered. The more creative plant designs utilized the process simulations in preparing the design including raw material requirements, energy requirements, list of major process equipment, and process economics (plant capital investment and product cost).

Industrial Support

By involving professional pedagogues, developers of best-practice chemical engineering curricula, neophyte and experienced students, and representatives from the vast local petrochemical industries of Southeast Texas, the project will improve the department's connections with the community in the best of practical educational modes. Local supporters include ExxonMobil, DuPont, Dow, and Huntsman Corporations. In addition to these, modeling and software companies and private entities are providing financial support, technical support, and personnel exchange programs. These are stakeholders in a program designed to teach chemical engineering fundamental principles, advanced tools including CAMS, and innovative problem analysis and solutions.

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